Many-body effects in the photo-emission of ferromagnets

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The one-step model of photoemission is used to investigate the angle-integrated spin-resolved valence band (VB) photoemission of the 3d-ferromagnets Fe, Co and Ni. This scheme has been implemented using a fully-relativistic version of the multiple scattering or KKR (Korringa-Kohn-Rostoker) formalism. This way in particular the influence of the spin-orbit coupling is properly accounted for allowing a very detailed discussion of the polarization dependence of the spectra. As is well known from previous work, especially on Ni, the VB-photoemission spectra clearly show the impact of many-body effects as e.g. the apparent shrinkage of the d-band width and the occurance of satellites. To account for these phenomena we used within the underlying electronic structure calculation a combination of local spin density approximation (LSDA) and dynamical mean field theory (DMFT), that results in an improved treatment of correlation effects compared to plain LSDA-based calculations. On the basis of this very powerful approach angle-integrated and spin-resolved VB-spectra have been calculated for circularly polarized light. Our theoretical results are compared to recent experimental spectra recorded at the ESRF. A comparison of LSDA- and LSDA+DMFT- based results to experiment clearly demonstrate the impact of correlation effects. Our theoretical and experimental results for a setup where the incoming photon beam is perpendicular to the intrinsic magnetization clearly show that the pure Fano-effect can be observed also in ferromagnets. The spectra for a setup where the photon beam is parallel to the magnetization is used to construct the so-called fundamental spectra. Application of the so-called sum rules leads to results for the spin and orbital moments that are in reasonable agreement with data stemming from direct calculations or other experiments.